Technische Universität Braunschweig

Institute for Computational Mathematics

Introduction to Model Order Reduction
A Tutorial

Matthias Bollhöfer
INRIA Sophia Antipolis , July 27, 2015

Outline

- **Model Order Reduction**
- **Proper Orthogonal Decomposition**
- **Balanced Truncation**
- **Moment Matching**
- **Conclusions**

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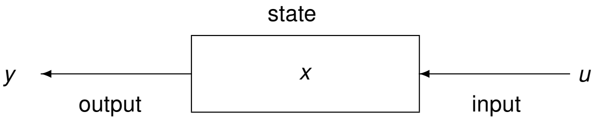
Objective of Model Order Reduction (MOR)



Dynamical system

$$\begin{aligned} \dot{x} &= Ax + Bu \\ y &= Cx + Du \end{aligned}$$

Laplace transformation, transfer function $\mathcal{H}(s)$

$$\begin{aligned} \mathcal{H}(s) &:= C(sI - A)^{-1}B + D \\ \hat{y}(s) &= \mathcal{H}(s)\hat{u} + \dots \end{aligned}$$

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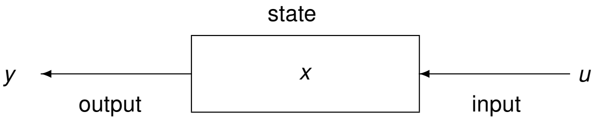

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Here most of the time $B, C^* \in \mathbb{R}^n$, single-input single-output case

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$$\mathcal{H}(s) = C(sI - A)^{-1}B + D, \quad \hat{\mathcal{H}}(s) = \hat{C}(sI - \hat{A})^{-1}\hat{B} + \hat{D}$$

$$\|\mathcal{H}(s) - \hat{\mathcal{H}}(s)\| \text{ small}$$

Example

Heat equation

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$$\frac{\partial T(x,0,t)}{\partial y} = \frac{\partial T(x,1,t)}{\partial y} = 0,\ \frac{\partial T(1,y,t)}{\partial x} = -\alpha(T(1,y,t) - T_e(y))$$

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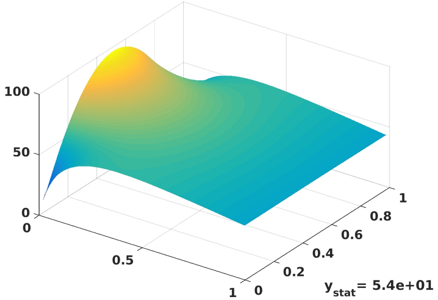
$E = \int_\Omega T\, dxdy$ output, total temperature

spatial discretization (FDM/FEM)

$$\begin{aligned} \dot{T}(t) &= -AT(t) + Bu(t) \\ E(t) &= CT(t) \end{aligned}$$

A sym. pos. def. rnk$B$ refers to dependence of u w.r.t. y



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Set $X = \left[\tilde{x}^{(1)}, \ldots, \tilde{x}^{(m)}\right]$.

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Euclidean scalar product $(v, w) = v^* M w$, find orthonormal basis $z^{(1)}, \ldots, z^{(r)}$ s.t.

$$\sum_{i=1}^{m} \|\tilde{x}^{(i)} - \sum_{j=1}^{r} \mu_{ij} z^{(j)}\|_M^2$$

is minimized.

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- $\mu_{ij} = (z^{(i)}, x^{(j)})$ (M-orthogonal projection)
- best rank–r approximation of X given by $M^{1/2}X = U\Sigma V^*$ (SVD), $Z_r = \left[z^{(1)}, \ldots, z^{(r)}\right] = M^{-1/2}U_r$, where U_r refers to the leading r columns of U (EMSY-Theorem).

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$$\boxed{\dot{a} = \hat{A}a + \hat{B}u,\ \tilde{y} = \hat{C}a + Du}$$

$\rightarrow$ solve reduced-order dynamical system for the Fourier coefficients $a_j(t)$.

Example

Heat equation

$$T_t = \kappa \Delta T \text{ in } \Omega = [0, 1]^2$$

$N = 100$ grid points in x-, y-direction $t_e = 10$, $M = 20$ time steps (snapshots)
SVD, $\sigma_1, \dots, \sigma_r \geqslant \tau \|X\|$
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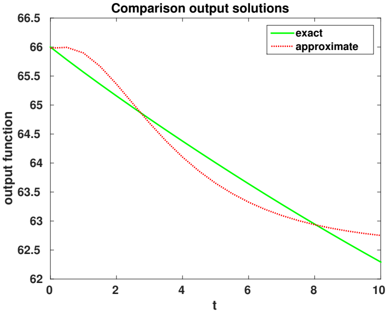

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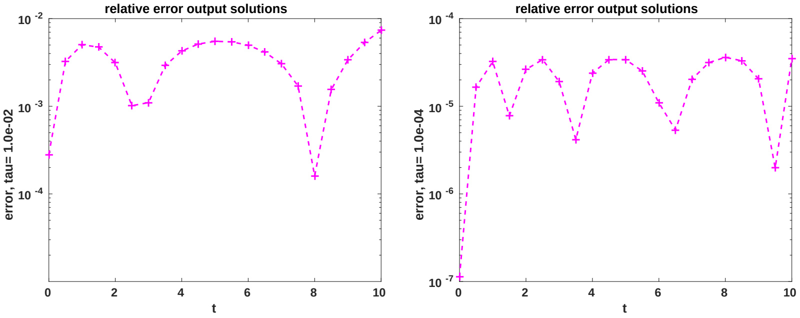

Remarks POD

- initial phase (offline phase) is expensive (computing snapshots, SVD)
- solving reduced order is almost for free (online phase)
- POD works well for problems like the heat equation (singular values of the analytic solution decay quadratically w.r.t. t)

$$T(x,y,t) \sim \sum_{l,m} \mu_{l,m} e^{-\kappa(l^2+m^2)\pi^2 t} \sin(l\pi x)\sin(m\pi y)$$

- POD leads to significantly higher rank for wave equations (singular values of the analytic solution decay linearly w.r.t. t)
- zero eigenvalues of the operator A on the imaginary axis (Maxwell, nullspace of the curl operator) severly interfere with POD.

Remarks POD

Variants of POD, e.g. affine-linear subspace

$$\underline{x} = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}, \quad D := X - \underline{x}\begin{pmatrix} 1 & \cdots & 1 \end{pmatrix}$$

Compute SVD of $M^{1/2}D = U\Sigma V^*$ and use for POD affine-linear model

$$\tilde{x} = \underline{x} + M^{-1/2}U_r a$$

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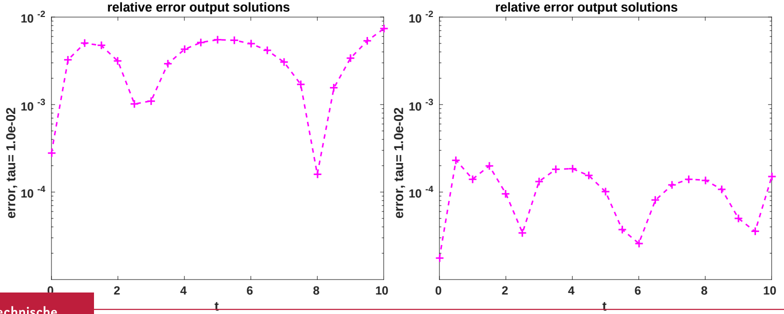
linear POD $\tau = 10^{-2}$, $r = 3$ versus affine-linear POD $\tau = 10^{-2}$, $r = 4$



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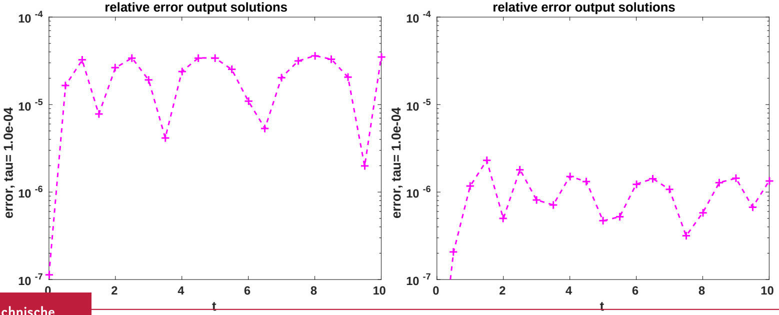

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The square roots of the eigenvalues of PQ are called Hankel singular values of the dynamical system

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We can construct T such that (A, B, C, D) is balanced!

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Partition the factors of the SVD $U\Sigma V^* = G$ as

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$$T_r := LU_1\Sigma_1^{-1/2},\quad W_r := R^* V_1\Sigma_1^{-1/2} \ \Rightarrow\ W_r^* T_r = I_r$$

(T_r, W_r are the leading r columns/rows of T, T^{-1})

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$$T_r := LU_1\Sigma_1^{-1/2},\quad W_r := R^* V_1\Sigma_1^{-1/2} \ \Rightarrow\ W_r^* T_r = I_r$$

(T_r, W_r are the leading r columns/rows of T, T^{-1})

Associated reduced order model:

$$\hat{A} := W_r^* A T_r,\ \hat{B} := W_r^* B,\ \hat{C} := C T_r,\ \hat{D} := D.$$

Benefit of Balancing the Dynamical System

How can we use the balancing decomposition for MOR?

Partition the factors of the SVD $U\Sigma V^* = G$ as

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Error bound $\|\hat{y} - y\|_{L_2} \leqslant \|\hat{\mathcal{H}} - \mathcal{H}\|_{H_\infty} \|u\|_{L_2} = 2(\sigma_{r+1} + \cdots + \sigma_n)\|u\|_{L_2}$

Balanced Truncation Algorithm

1. Compute a low-rank approximation $L_r L_r^* \approx P$ directly from

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The ADI Method

Objective: Solve $AP + PA^* + BB^* = 0$

Alternating direction implicit method (ADI): Given some P_{j-1} and shift τ_j, compute

$$(\tau_j I + A) P_{j-\frac{1}{2}} \stackrel{!}{=} -BB^* + P_{j-1}(\tau_j I - A)^*$$

$$P_j(\tau_j I + A)^* \stackrel{!}{=} -BB^* + (\tau_j I - A) P_{j-\frac{1}{2}}$$

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- Convergence well-understood in the SPD case, there optimal shifts are known
- General case more complicate
- Here we want to exploit $P_j = L_j L_j^*$ explicitly
  $\longrightarrow$ low-rank Smith method, low-rank Cholesky-factor ADI

Low-Rank Cholesky-Factor ADI Method

Computing an approximate low-rank solution $L_r L_r^*$ of $AL_r L_r^* + L_r L_r^* A^* + BB^* \approx 0$

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$$
\begin{aligned}
Z_i &:= \frac{\sqrt{-2\tau_i}}{\sqrt{-2\tau_{i-1}}} \left[Z_{i-1} - (\tau_i + \bar{\tau}_{i-1}) (\tau_i I + A)^{-1} Z_{i-1} \right] \\
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Remark. Shift parameters are essential, optimal values only known if $-A$ is s.p.d.
“error” usually measured by changes from $L_{i-1} \to L_i$.
each update i increases $L_{i-1} \to L_i$ by rank$B$

Example Balanced Truncation

Heat equation

$$T_t = \kappa \Delta T \text{ in } \Omega = [0, 1]^2$$

$N = 100$ grid points in x-, y-direction $t_e = 10$, $M = 20$ time steps
Low-Rank Cholesky-Factor ADI using 0.1τ
$\tau = 10^{-2} \Rightarrow 23/13$ ADI steps, $\tau = 10^{-4} \Rightarrow 40/29$ ADI steps
SVD of $G = L_r^* R_r^*$, $\sigma_1, \dots, \sigma_r \geqslant \tau \|X\|$
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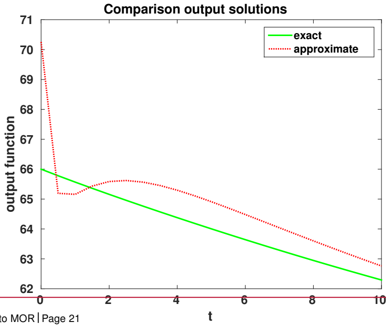

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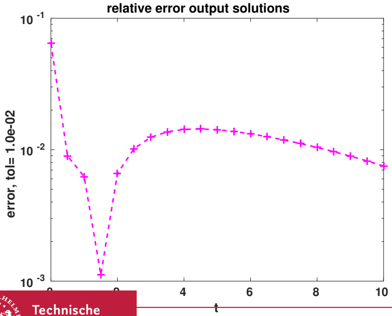

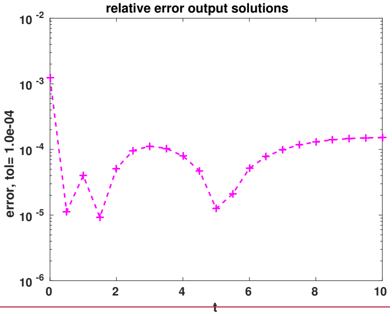

Remarks Balanced Truncation

- BT yields error bounds!
- $\sigma(A) \in \mathbb{C}^-$ essential (similar situation as for POD)
- BT can be generalized to descriptor systems $E\dot{x} = Ax + Bu$
- Additional properties such as passivity can be preserved by modifying BT (passivity: $\mathcal{H}(s)$ is analytic, $\mathcal{H}(s) + \mathcal{H}(\bar{s})^*$ is positive semidefinite f.a. $s \in \mathbb{C}^+$)

Outline

- Model Order Reduction
- Proper Orthogonal Decomposition
- Balanced Truncation
- **Moment Matching**
- Conclusions

Moment Matching-Based Model Order Reduction

Dynamical system

$$\begin{aligned} \dot{x} &= Ax + Bu, \\ y &= Cx + Du, \end{aligned}$$

Transfer function

$$\mathcal{H}(s) = C(sI - A)^{-1}B$$

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$$\mathcal{H}(s) = \sum_{p=0}^{\infty} Z_0^{(p)}(s - s_0)^p, \text{ where } Z_0^{(p)} = -C(A - s_0 I)^{-p-1}B$$

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$X_0^{(p)} := -(A - s_0 I)^{-p-1}B$ input moments, Taylor coefficients $Z_0^{(p)}$ output moments.
$Y_0^{(p)} := -C(A - s_0 I)^{-p-1}$

Elementary Considerations

Suppose that A is simple, $T^{-1}AT = \Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$, $Re(\lambda_j) < 0$.

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- matching eigenvectors/eigenvalues close to the imaginary axis advantageous
- Taylor expansion of $\mathcal{H}(s)$ sensitive w.r.t. expansion point s_0
- Often applications only require $\max_{\omega \in [f_{\min}, f_{\max}]} \|\hat{\mathcal{H}}(2\pi i \omega) - \mathcal{H}(2\pi i \omega)\|_\infty$ to be small

Krylov Subspace Methods

Krylov subspace

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$$(Y_0^{(p)})^* = (A^* - \bar{s}_0 I)^{-p-1} C^* \in \mathcal{K}_{p+1}((s_0 I - A)^{-*}, C_0^*), \text{ where } C_0^* = (A - s_0 I)^{-*} C^*.$$

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Main idea of moment matching methods:
Compute T_r and/or W_r from $\mathcal{K}_r((s_0 I - A)^{-1}, B_0)$, $\mathcal{K}_r((s_0 I - A)^{-*}, C_0^*)$ s.t. $W_r^* T_r = I$

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Moment Matching Methods

Consequences

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- If $T_r \in \mathcal{K}_r((s_0 I - A)^{-1}, B_0)$ and W_r s.t. $W_r^* T_r = I$, then $t \geqslant r$
- If $W_r \in \mathcal{K}_r((s_0 I - A)^{-*}, C_0^*)$ and T_r s.t. $W_r^* T_r = I$, then $t \geqslant r$
- If $T_r \in \mathcal{K}_r((s_0 I - A)^{-1}, B_0)$ and $W_r \in \mathcal{K}_r((s_0 I - A)^{-*}, C_0^*)$ $W_r^* T_r = I$, then $t \geqslant 2r$.

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Lanczos-type method (Padé via Lanczos)

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Generate dual bases T_r of $\mathcal{K}_r((s_0 I - A)^{-1}, B_0)$ <u>and</u> W_r of $\mathcal{K}_r((s_0 I - A)^{-*}, C_0^*)$

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$$\underline{L}_r = \left[\begin{array}{cccc} l_{11} & l_{12} & & 0 \\ l_{21} & l_{22} & l_{23} & \\ & \ddots & \ddots & \ddots \\ 0 & & l_{r-1,r-2} & l_{r-1,r-1} \\ \hline 0 & & & l_{r,r-1} \end{array}\right], \quad \underline{\hat{L}}_r = \left[\begin{array}{cccc} \bar{l}_{11} & \bar{l}_{21} & & 0 \\ \bar{l}_{12} & \bar{l}_{22} & \bar{l}_{32} & \\ & \ddots & \ddots & \ddots \\ 0 & & \bar{l}_{r-2,r-1} & \bar{l}_{r-1,r-1} \\ \hline 0 & & & \bar{l}_{r-1,r} \end{array}\right].$$

Krylov Subspace Methods — Lanczos (PVL)

$t := (s_0 I - A)^{-1} B$, $w := (s_0 I - A)^{-*} C^*$
$T_1 := t/\|t\|$, $W_1 = w/(T_1^* w)$

$t := (s_0 I - A)^{-1} B$, $w := (s_0 I - A)^{-*} C^*$
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$l_{01} = l_{10} := 0$

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$l_{01} = l_{10} := 0$
For $i = 1, 2, \dots, r-1$
  $t := (s_0 I - A)^{-1} T_i$
  $l_{ii} := W_i^* t$
  $t := t - T_i l_{ii} - T_{i-1} l_{i-1,i}$
  $l_{i+1,i} := \|t\|$, $T_{i+1} := t / l_{i+1,i}$

  $w := (s_0 I - A)^{-*} W_i$
  $w := w - W_i \bar{l}_{ii} - W_{i-1} \bar{l}_{i,i-1}$
  $l_{i,i+1} := w^* T_i$, $W_{i+1} := w / \bar{l}_{i,i+1}$

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Arnoldi-type method

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Generate orthonormal basis T_r of $\mathcal{K}_r((s_0 I - A)^{-1}, B_0)$

We obtain $(s_0 I - A)^{-1} T_{r-1} = T_r \underline{H}_r$, where $T_r^* T_r = I$ and

$$\underline{H}_r = \left[\begin{array}{cccc} h_{11} & \cdots & \cdots & h_{1,r-1} \\ h_{21} & h_{22} & & \vdots \\ & \ddots & \ddots & \vdots \\ 0 & & h_{r-1,r-2} & h_{r-1,r-1} \\ \hline 0 & & & h_{r,r-1} \end{array}\right].$$

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  For $j = 1, 2, \ldots, i$
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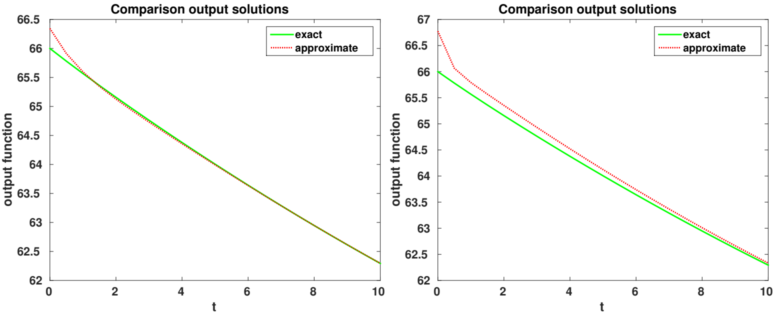
PVL ($r = 3$) versus Arnoldi ($r = 3$)



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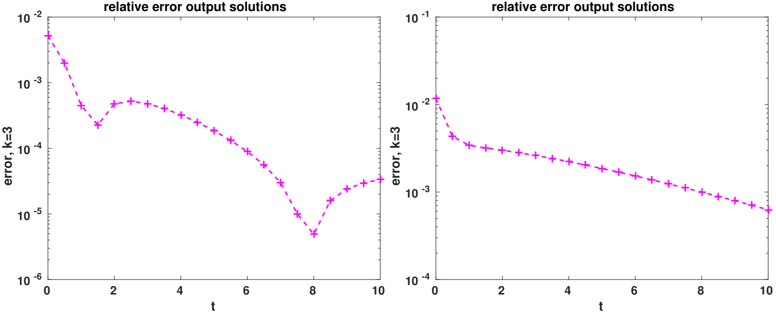

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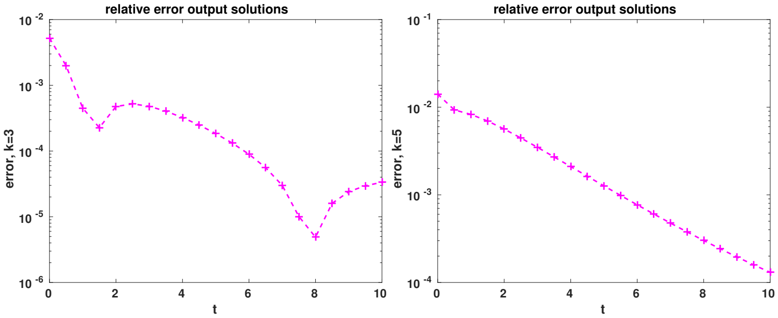

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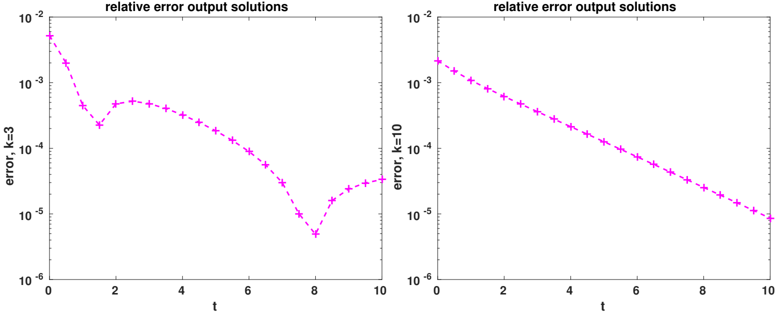

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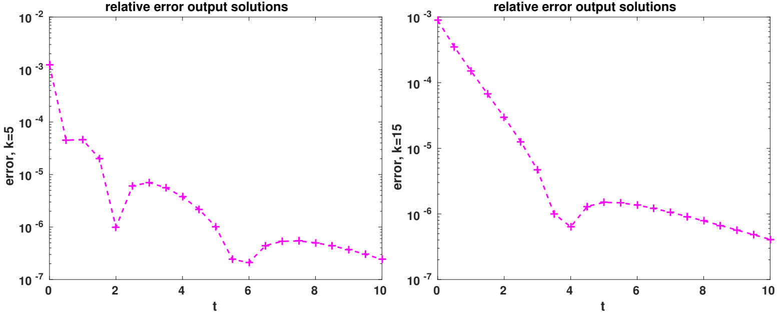
PVL ($r = 5$) versus Arnoldi ($r = 15$)



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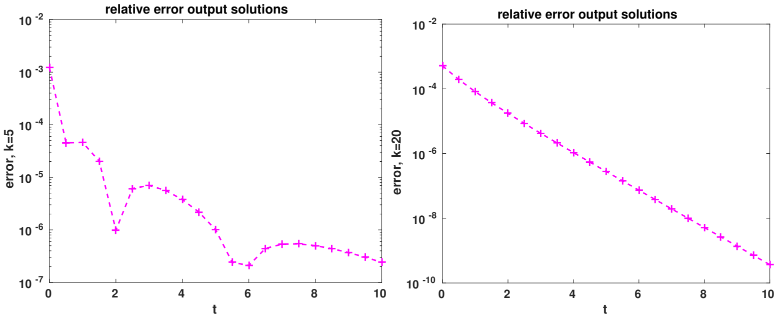

Remarks Krylov Subspace Methods

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- Arnoldi more stable, either B or C^* is taken into acount, stable, preserves symmetry

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- Krylov subspace methods are extremeley sensitive to the choice of s_0, location of eigenvalues of A is helpful (e.g. real and negative), frequency range as well
- shift s_0 on the imaginary axis, usually complex-valued matrices T, W

Rational Krylov Subspace Methods

- Use multiple Taylor expansions at $s_1, \ldots, s_l$

$$\mathcal{H}(s) = \sum_{p=0}^{\infty} Z_j^{(p)} (s - s_j)^p, \; j = 1, \ldots, l$$

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and/or possibly basis W_r (such that $W_r^* T_r = I$) for the Krylov subspaces

$$\sum_{j=1}^{l} \mathcal{K}_{r_j}((s_j I - A)^{-*}, C_j^*), \text{ where } C_j = (s_j I - A)^{-*} C^*$$

$$r = r_1 + \cdots + r_l$$

Rational Arnoldi Methods

Lemma (Partial Fraction Decomposition)

Suppose that $s_i \neq s_j$, then

$$(s_i I - A)^{-1} \cdot (s_j I - A)^{-p+1} B_j \in \mathcal{K}_p((s_j I - A)^{-1}, B_j) + \mathcal{K}_1((s_i I - A)^{-1}, B_i)$$

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- $\Rightarrow$ mixing inverses with different shifts leads to a separate sum of Krylov subspaces, no “mixed powers of inverses”
- We may run the Arnoldi method with shifts $s_1, \ldots, s_l$ simultaneously, e.g., one shift after another or cyclically

Example Rational Arnoldi Method

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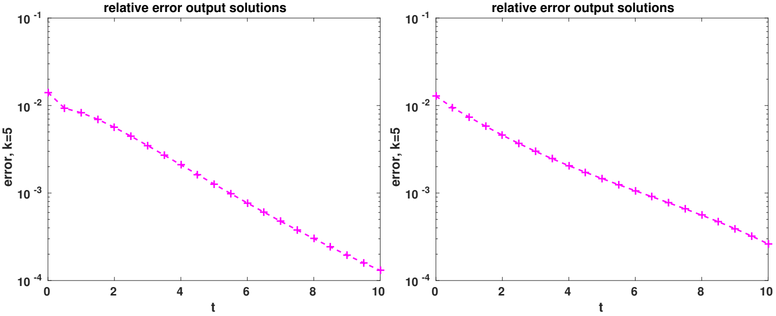

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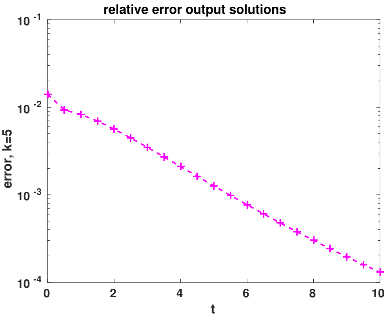

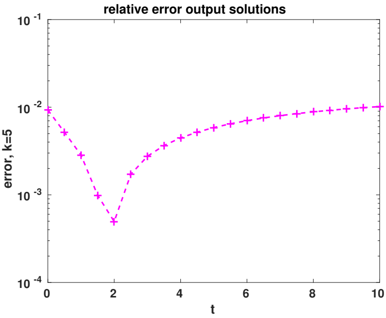

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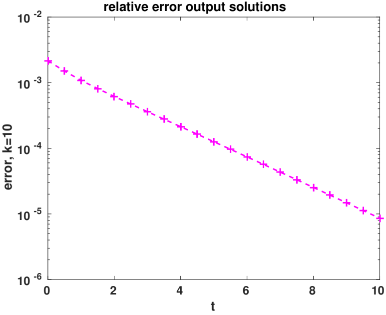

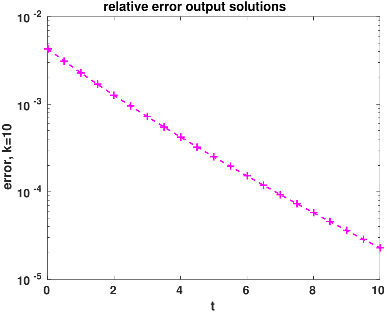

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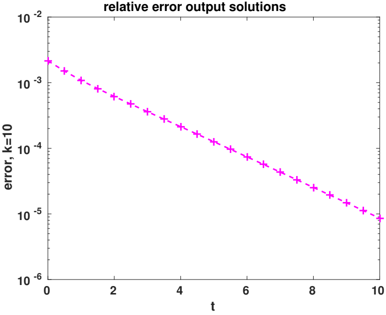

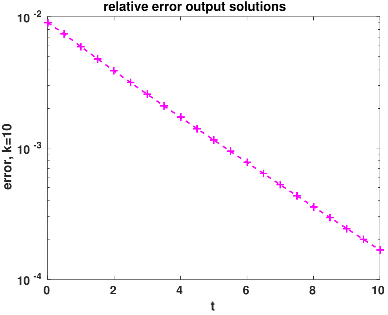

Remarks Rational Arnoldi Method

- Choice of multiple shifts not clear in advance, sometimes one shift is enough
- Multiple shifts may reduce the error $\|\hat{\mathcal{H}}_{r_l}(s) - \hat{\mathcal{H}}_{r_{l+1}}(s)\| / \|\hat{\mathcal{H}}_{r_{l+1}}(s)\|$ between two subsequent rational Arnoldi calls more uniformly
- Adaptive strategies to select s_j exist
- Multiple shifts require more *LU* decompositions

Technische Universität Braunschweig

Outline

- Model Order Reduction
- Proper Orthogonal Decomposition
- Balanced Truncation
- Moment Matching
- **Conclusions**

Conclusions

- Three different approaches to perform model order reduction presented
- Discussion here only simplified!
- no clear winner, problem-dependent
- POD: use SVD of a snapshot sequence,
  BT: use low-rank approximation of the associated Gramians
  Moment Matching: build bases of the associated Krylov subspace
- Many additional topics to be discussed (generalizations to $E\dot{x} = Ax + Bu$, error estimates for Krylov-type methods, numerical solvers for solving the shifted systems, parametrized systems, time-dependent systems, nonlinear systems,. . .)